Cas react

FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 14:29:41 ON 25 OCT 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 OCT 2005 HIGHEST RN 865981-77-7
DICTIONARY FILE UPDATES: 24 OCT 2005 HIGHEST RN 865981-77-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

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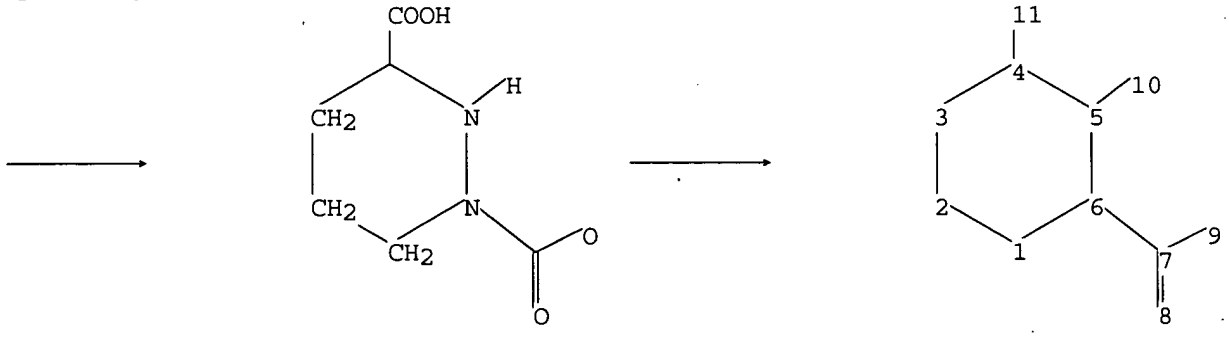
**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************
```

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10826031pp.str



chain nodes :
7 8 9 10 11
ring nodes :
1 2 3 4 5 6
chain bonds :

<10/25/2005> Habte

4-11 5-10 6-7 7-8 7-9
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 6-7 7-8 7-9
exact bonds :
4-11 5-10

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS
fragments assigned product role:
containing 1

L1 STRUCTURE UPLOADED

=> file casreact

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.43	0.64

FILE 'CASREACT' ENTERED AT 14:30:15 ON 25 OCT 2005
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTENT:1840 - 23 Oct 2005 VOL 143 ISS 17

New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*
* CASREACT now has more than 9.2 million reactions *
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> s l1
SAMPLE SEARCH INITIATED 14:30:29 FILE 'CASREACT'
SCREENING COMPLETE - 19 REACTIONS TO VERIFY FROM 1 DOCUMENTS

100.0% DONE 19 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

<10/25/2005> Habte

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                          BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:        119 TO      641
PROJECTED ANSWERS:                0 TO        0

L2             0 SEA SSS SAM L1 (      0 REACTIONS)

=> s l1 sss full
FULL SEARCH INITIATED 14:30:57 FILE 'CASREACT'
SCREENING COMPLETE -    334 REACTIONS TO VERIFY FROM       19 DOCUMENTS

100.0% DONE     334 VERIFIED      21 HIT RXNS                      4 DOCS
SEARCH TIME: 00.00.01

L3             4 SEA SSS FUL L1 (     21 REACTIONS)

=> d fhit ibib abs tot
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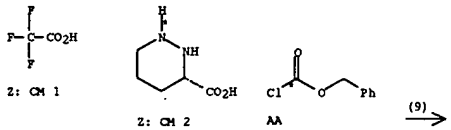
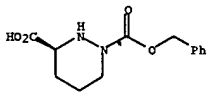
L3 ANSWER 1 OF 4 CASREACT COPYRIGHT 2005 ACS on STN

RX(9) OF 122 ...Z + AA ===> AB...





AB
YIELD 40%

RX(9) RCT Z 156699-40-0, AA 501-53-1
RGT AC 1310-73-2 NaOH
PRO AB 65632-62-4
SOL 7732-18-5 Water, 108-88-3 PhMe
ACCESSION NUMBER: 140:357083 CASREACT
TITLE: Stereochemical Definition and Chirospecific Synthesis of the Peptide Deformylase Inhibitor Sch 382583
AUTHOR(S): Coats, Reed A.; Lee, Sheng-Lian; Davis, Kari A.; Patel, Kanu M.; Rhoads, Elaine K.; Howard, Michael H.
CORPORATE SOURCE: Stine-Haskell Research Center, DuPont Crop Protection, Newark, DE, 19711, USA
SOURCE: Journal of Organic Chemistry (2004), 69(5), 1734-1737 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The recently reported natural product Sch 382583 (I), an inhibitor of peptide deformylase, has been synthesized in 16 steps from com. available starting materials. The three chiral centers were set by a combination of chiral auxiliary and chiral pool approaches. The succinate II and

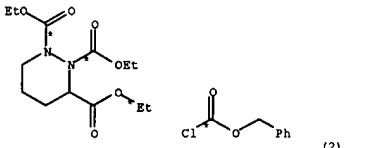
L3 ANSWER 1 OF 4 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

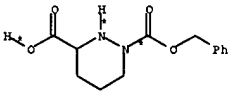
piperazic acid III moieties were obtained by Evans oxazolidinone imide enolate alkylation and hydrazination/cyclization, resp., and the aminohexanone side chain IV was prepd. via Grignard substitution of the Weinreb amide derived from L-valine. Spectroscopic data for the resulting synthetic material, compared with the data reported for the natural product, established that the previously unassigned valine ketone stereocenter (C-4) has the S-configuration.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 4 CASREACT COPYRIGHT 2005 ACS on STN

RX(2) OF 3 ...C + I ===> J





J
YIELD 81%

RX(2) RCT C 150927-67-6

STAGE(1)
RGT K 1310-58-3 KOH
SOL 71-36-3 BuOH

STAGE(2)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(3)
RCT I 501-53-1
RGT M 1310-73-2 NaOH
SOL 108-88-3 PhMe, 7732-18-5 Water

STAGE(4)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water

PRO J 72120-54-8
ACCESSION NUMBER: 135:137513 CASREACT
TITLE: Process for preparing piperazic acid and its derivatives from the cyclocondensation reaction of 2,5-dihalopentanoate esters with dialkyl hydrazodicarboxylates
INVENTOR(S): Brieden, Walter; O'Murchu, Colm
PATENT ASSIGNEE(S): Lonza A.-G., Switz.

L3 ANSWER 2 OF 4 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

SOURCE: PCT Int. Appl., 14 pp. CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001056997	A1	20010809	WO 2001-EP1159	20010202

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, US, US
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: EP 2000-102420 20000204
US 2000-203936P 20000512
OTHER SOURCE(S): MARPAT 135:137513
GI

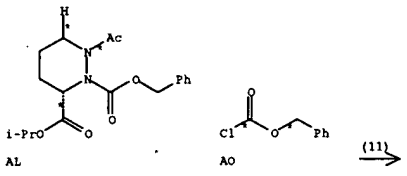
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Piperazic acid derivs. [I; R1 = C1-20 alkyl; R2 = H, C1-6 alkyl, C1-6 haloalkyl, C1-6 alkoxy, allyloxy, 2,2,2-trichloroethoxy, 2-iodoethoxy, (un)substituted Ph, benzyloxy, 4-methoxybenzyloxy, 2,4-dimethoxybenzyloxy] (e.g., tri-Et hexahydro-1,2,3-pyridazinetricarboxylate) are prepared in high yield and selectivity by the cyclocondensation reaction of a 2,5-dihalopentanoate esters XCH2CH2CH2CHXCO2R1 (X = Br, Cl; e.g., Et 2,5-dibromopentanoate) in the presence of a base (e.g., sodium hydride) and a hydrazodicarboxylate esters R2CONHNHCOR2 (e.g., di-Et hydrazodicarboxylate), followed by basic (e.g., aqueous KOH solution reflux) removal of the blocking groups to give alkali piperazic acid salts (II; M = alkali metal; e.g., piperazic acid potassium salt) followed by amidation with chloroformate esters R3O2CCl (R3 = alkyl, allyl, 2,2,2-trichloroethyl, 2-iodoethyl, benzyl, 4-methoxybenzyl, 2,4-dimethoxybenzyl; e.g., benzyl chloroformate) to form piperazinic acid derivs. [III; N1-(benzyloxycarbonyl)piperazic acid].

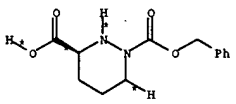
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 4 CASREACT COPYRIGHT 2005 ACS on STN

RX(11) OF 87 ...AL + AO ===> AP



AL AO (11)



AP
YIELD 61%

RX(11) RCT AL 176237-47-1

STAGE(1)
RGT H 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH

STAGE(2)
RGT Y 7647-01-0 HCl
SOL 7732-18-5 Water

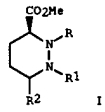
STAGE(3)
RCT AO 501-53-1

PRO AP **65632-62-4**
NTE LAST STAGE AT PH 7

ACCESSION NUMBER: 125:11384 CASREACT
TITLE: Amino acids and peptides. Part 100. Enantioselective syntheses of (R)- and (S)-hexahydropyridazine-3-carboxylic acid derivatives
AUTHOR(S): Schmidt, Ulrich; Braun, Christine; Sutoris, Heinz

L3 ANSWER 3 OF 4 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

CORPORATE SOURCE: Inst. Org. Chemie Isotopenforschung, Univ. Stuttgart, Stuttgart, D-70569, Germany
SOURCE: Synthesis (1996), (2), 223-9
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

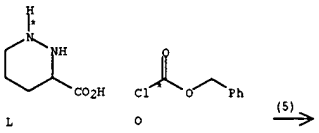


I

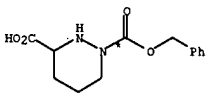
AB Pyridazine-3-carboxylic acids e.g. I (R = CO2CH2Ph, R1, R2 = H or bond; R, R2 = H, R1 = CO2CH2Ph) were prepared via ring closure of α-hydrazino- and δ-hydrazinopentanoates. Either optically active glutamic acid or an enantioselective catalytic hydrogenation was used to generate the chiral center. The numerous optically active intermediates are valuable starting materials for the synthesis of other unusual amino acids.

L3 ANSWER 4 OF 4 CASREACT COPYRIGHT 2005 ACS on STN

RX(5) OF 15 ...L + O ===> P



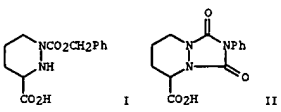
L O (5)



P
YIELD 66%

RX(5) RCT L 32750-52-0, O 501-53-1
RGT Q 1310-73-2 NaOH
PRO P **72120-54-8**
SOL 7732-18-5 Water, 108-88-3 PhMe

ACCESSION NUMBER: 111:23466 CASREACT
TITLE: Preparation of 1-(benzyloxycarbonyl)hexahydro-3-pyridazinecarboxylic acid, a protected piperazic acid
AUTHOR(S): Adams, C. E.; Aguilar, D.; Hertel, S.; Knight, W. H.; Paterson, J.
CORPORATE SOURCE: Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA
SOURCE: Synthetic Communications (1988), 18(18), 2225-31
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I II

AB 4-Phenylurazole was employed in a multistep synthesis of the title acid (I). The urazole was dehydrogenated, the product underwent a Diels-Alder reaction with CH2:CHCH:CHCO2H, and the adduct obtained was hydrogenated to bicyclic compound II. II was hydrolyzed by KOH, and subsequent acylation

L3 ANSWER 4 OF 4 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

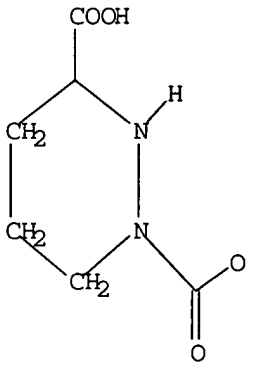
with ClCO2CH2Ph gave I.

4-11 5-10 6-7 7-8 7-9
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 6-7 7-8 7-9
exact bonds :
4-11 5-10

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 14:25:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 8 TO 329
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 14:25:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 177 TO ITERATE

100.0% PROCESSED 177 ITERATIONS 7 ANSWERS

SEARCH TIME: 00.00.01

L3 7 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	161.54

FILE 'CAPLUS' ENTERED AT 14:26:07 ON 25 OCT 2005
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FILE COVERS 1907 - 25 Oct 2005 VOL 143 ISS 18
FILE LAST UPDATED: 24 Oct 2005 (20051024/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3
L4 27 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:56771 CAPLUS
DOCUMENT NUMBER: 142:155962
TITLE: Catalytic cyclocondensation process for the production of 1,2-disubstituted-hexahydropyridazine-3-carboxylic acids and their esters from N,N'-disubstituted hydrazines and 2,5-dihalovaleric acids
INVENTOR(S): Nerenz, Frank; Bartels, Guenter; Kanschick-Conradsen, Andreas
PATENT ASSIGNEE(S): Honeywell Specialty Chemicals Seelze GmbH, Germany
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10328888	A1	20050120	DE 2003-10328888	20030626
WO 2005028449	A1	20050331	WO 2004-EP5284	20040517

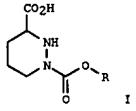
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: DE 2003-10328888 A 20030626
US 2003-505470P P 20030924
OTHER SOURCE(S): CASREACT 142:155962; MARPAT 142:155962
AB A cyclocondensation process for the production of 1,2-disubstituted-hexahydropyridazine-3-carboxylic acids (e.g., Me 1,2-dibenzyloxycarbonylhexahydropyridazine-3-carboxylate) and their esters from N,N'-disubstituted hydrazines (e.g., N,N'-dibenzyloxycarbonylhydrazine) and 2,5-dihalovaleric acids (e.g., Me 2,5-dibromovalerate) in the presence of phase-transfer catalysts (e.g., NaOH in the presence of Me tributylammonium chloride) is described.
IT 827602-71-1P 827602-73-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(catalytic cyclocondensation process for the production of 1,2-disubstituted-hexahydropyridazine-3-carboxylic acids and their esters from N,N'-disubstituted hydrazines and 2,5-dihalovaleric acids)
RN 827602-71-1 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:875976 CAPLUS
DOCUMENT NUMBER: 141:350183
TITLE: Process for the preparation of hexahydropyridazine-3-carboxylic acid derivatives via cyclocondensation of dihaloalkylcarboxylate with hydrazinedicarboxylate
INVENTOR(S): Lhermitter, Herve; Vincent, Charles-Henri; Picherit, Christian
PATENT ASSIGNEE(S): Isochem, Fr.
SOURCE: Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1468993	A1	20041020	EP 2004-290935	20040408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
FR 2853901	A1	20041022	FR 2003-4763	20030416
FR 2853901	B1	20050617		
CA 2463185	AA	20041016	CA 2004-2463185	20040414
US 2004210053	A1	20041021	US 2004-826031	20040415
JP 2004315535	A2	20041111	JP 2004-121089	20040416

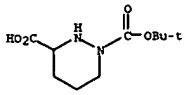
PRIORITY APPLN. INFO.: FR 2003-4763 A 20030416
OTHER SOURCE(S): MARPAT 141:350183
GI



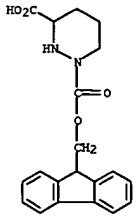
I

AB The invention is related to a process for preparation of hexahydropyridazine-3-carboxylic acids I by cyclocondensation of dihaloalkylcarboxylate of formula R3-(CH2)3-(CHR3)-CO2R2 with hydrazinedicarboxylate of formula RO-CO-NH-NH-CO-OR in the presence of a base (pK ≥ 8.5) and a ketone as organic solvent, and selective deprotection of the in-situ formed tricarboxylate in aqueous basic media [R = (un)substituted (un)saturated alkyl, (un)substituted aralkyl, aryl; R2 = (un)substituted alkyl; R3 = halo, nucleofuge]. The advantages include simple purification, rapid and economical one-step process. Thus, 1,2-(dibenzyloxycarbonyl)hydrazine reacted with Me 2,5-dibromovalerate in the presence of tetrabutylammopnium bromide, K2CO3 and acetone at reflux for 24 h, treatment with 30% NaOH solution at 40° for 5-7 h, and acidulation with HCl to pH = 1 gave the acid I (R = Bn).
IT 72120-54-8P, 1-(Benzyloxycarbonyl)hexahydropyridazine-3-carboxylic

L4 ANSWER 1 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

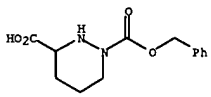


RN 827602-73-3 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(9H-fluoren-9-ylmethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

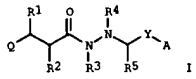
L4 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
acid
RL: IMF (Industrial manufacture); PREP (Preparation)
(product; prepn. of hexahydropyridazine-3-carboxylic acid derivs. via cyclocondensation of dihaloalkylcarboxylate with hydrazinedicarboxylate)
RN 72120-54-8 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:550932 CAPLUS
DOCUMENT NUMBER: 141:106199
TITLE: Preparation of novel hydroxamic acid and N-formylhydroxylamine derivatives as antibacterial agents
INVENTOR(S): East, Stephen Peter; Bragg, Ryan Ashley; Taylor, Steven
PATENT ASSIGNEE(S): Vernalis Oxford Ltd., UK
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056751	A1	20040708	WO 2003-GB5407	20031211
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1572630	A1	20050914	EP 2003-780379	20031211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.: GB 2002-29673 A 20021219
WO 2003-GB5407 W 20031211
OTHER SOURCE(S): MARPAT 141:106199
GI



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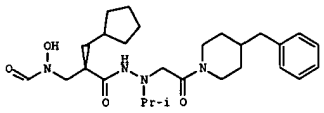
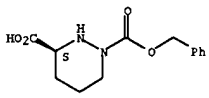


II

L4 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

AB The title compds. [I; Q = N(OH)CHO or CONH(OH); Y = CO, CS, SO, SO2; R1 = H, alkyl, alkyl substituted by one or more halogen atoms, or, except when Q = N(OH)CHO, OH, alkoxy, alkenyloxy, halo, NH2, alkylamino, or dialkylamino; R2 = (un)substituted alkyl, alkyl-O-alkyl, alkyl-S-alkyl, cycloalkylalkyl, arylalkyl, heterocyclylalkyl, etc.; R3, R5 = H, (un)substituted alkyl; or R3 and R5 taken together with the carbon and nitrogen atoms to which they are resp. attached form a saturated heterocyclic ring of 5-7 ring atoms, which may be fused to a second carbocyclic or heterocyclic ring, either of which rings may optionally be substituted; R4 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, etc.; A = a primary, secondary or tertiary amino group or a group R6, OR6 (wherein R6 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, etc.)], useful for treating bacterial infections, were prepared E.g., a multi-step synthesis of (2R)-II, was given. The compds. I were tested for their antibacterial activity. MIC ranges were given for representative compds. I. A pharmaceutical or veterinary composition comprising the compound I is claimed.
IT 65632-62-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel hydroxamic acid and N-formylhydroxylamine derivs. as antibacterial agents)
RN 65632-62-4 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



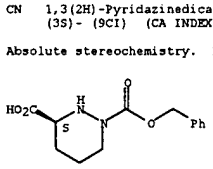
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:82567 CAPLUS
DOCUMENT NUMBER: 140:357083
TITLE: Stereochemical Definition and Chirospecific Synthesis of the Peptide Deformylase Inhibitor Sch 382583
AUTHOR(S): Coats, Reed A.; Lee, Sheng-Lian; Davis, Kari A.; Patel, Kanu M.; Rhoads, Elaine K.; Howard, Michael H.
CORPORATE SOURCE: Stine-Haskell Research Center, DuPont Crop Protection, Newark, DE, 19711, USA
SOURCE: Journal of Organic Chemistry (2004), 69(5), 1734-1737
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:357083
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The recently reported natural product Sch 382583 (I), an inhibitor of peptide deformylase, has been synthesized in 16 steps from com. available starting materials. The three chiral centers were set by a combination of chiral auxiliary and chiral pool approaches. The succinate II and piperazic acid III moieties were obtained by Evans oxazolidinone imide enolate alkylation and hydrazination/cyclization, resp., and the aminohexanone side chain IV was prepared via Grignard substitution of the Weinreb amide derived from L-valine. Spectroscopic data for the resulting synthetic material, compared with the data reported for the natural product, established that the previously unassigned valine ketone stereocenter (C-4) has the S-configuration.
IT 65632-62-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereochem. definition and chirospecific synthesis of the peptide deformylase inhibitor Sch 382583)
RN 65632-62-4 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



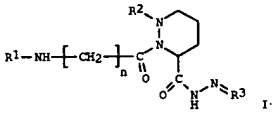
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:990976 CAPLUS
DOCUMENT NUMBER: 140:42190
TITLE: Combinatorial libraries of hydrazides and hydrazones of pyridazine-3-carboxylic acid, their use as drugs, particularly as inhibitors of cathepsin K, pharmaceutical compositions containing them, and methods for their preparation
INVENTOR(S): Bhatnagar, Neerja; Broto, Pierre; Gourvest, Jean Francois; Mauger, Jacques
PATENT ASSIGNEE(S): Aventis Pharma Sa, Fr.
SOURCE: Fr. Demande, 55 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2840898	A1	20031219	FR 2002-7346	20020614
FR 2840898	B1	20040827		
CA 2489447	AA	20031224	CA 2003-2489447	20030612
WO 2003106431	A2	20031224	WO 2003-FR1770	20030612
WO 2003106431	A3	20040408		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1515953	A2	20050323	EP 2003-760021	20030612
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003012127	A	20050329	BR 2003-12127	20030612
JP 2005530823	T2	20051013	JP 2004-513264	20030612
US 2005215553	A1	20050929	US 2004-9249	20041210

PRIORITY APPLN. INFO.: FR 2002-7346 A 20020614
WO 2003-FR1770 W 20030612
OTHER SOURCE(S): MARPAT 140:42190
GI

L4 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



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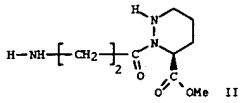


II

AB Combinatorial libraries of compds. I [wherein n = 0-6; R1 = CO(CH2)mR, CONH(CH2)mR, CSNH(CH2)mR, SO2(CH2)mR; m = 0-6, with optional presence of a double bond when m > 2; R = H (when m ≠ 0), OH, SH, alkoxy, aryloxy, aralkoxy, cycloalkyl, (un)substituted (un)saturated hetero(bi)cyclic, (un)substituted aryl, aralkyl; NH2 and derivs.; R2 = R1 or H; N R3 = N-R3, N:R3; R3 = R1 when NR3 is N-R3, and R when NR3 is N:R3; their isomers, racemates, enantiomers, diastereomers and their addition salts with acids or bases] were prepared for treatment of disorders linked to proteases and kinases, and particularly those in which cathepsin K is involved. For example, a combinatorial library of 810 (9x9x10) of I (n =2, N-R3 single bond) was prepared on solid support by a first acylation of II (preparation given) at the primary amino group, a second acylation of II at the pyridazine-N, hydrazinolysis , and a third acylation of the hydrazide. II was prepared from Cbz-protected hexahydropyridazin-3-carboxylic acid and Cbz-β-alanine. I inhibited cathepsin K (no data). I are useful for treatment of cardiovascular diseases, cancers, CNS disorders, inflammatory diseases, infectious diseases, and bone disorders.

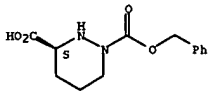
IT **65632-62-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of combinatorial libraries of hydrazides and hydrazones of pyridazinecarboxylic acid as inhibitors of cathepsin K)

RN 65632-62-4 CAPLUS

CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L4 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

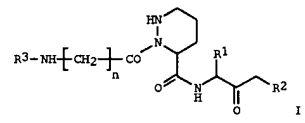
L4 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:879245 CAPLUS
DOCUMENT NUMBER: 139:364945
TITLE: New pyridazine-3-carboxylic acid derivatives, their use as drugs, particularly as inhibitors of cathepsin K, pharmaceutical compositions containing them, and methods for their preparation
INVENTOR(S): Bhatnagar, Neerja; Gourvest, Jean Francois; Mauger, Jacques
PATENT ASSIGNEE(S): Aventis Pharma SA, Fr.
SOURCE: Fr. Demande, 65 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2839309	A1	20031107	FR 2002-5573	20020503
FR 2839309	B1	20040723		
CA 2485083	AA	20031120	CA 2003-2485083	20030429
WO 2003095433	A1	20031120	WO 2003-FR1335	20030429
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
BR 2003004666	A	20040720	BR 2003-4666	20030429
EP 1503991	A1	20050209	EP 2003-749907	20030429
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005529147	T2	20050929	JP 2004-503450	20030429
US 2005171346	A1	20050804	US 2004-979679	20041102
PRIORITY APPLN. INFO.:			FR 2002-5573 A	20020503
			WO 2003-FR1335 W	20030429

OTHER SOURCE(S): MARPAT 139:364945
GI

L4 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



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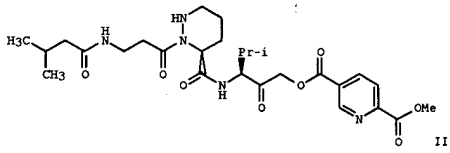


II

AB The invention provides title compds. I, chemical libraries thereof, a method of preparation of the compds., and their use as drugs [wherein: n = 0-6; R1 = (un)substituted alkyl, aryl, aralkyl, (un)saturated hetero(bi)cyclic; R2 = diazo, halo, OH, O(CH2)mR, S(CH2)mR, OCO(CH2)mR, NRR'; m = 0-6, with optional presence of a double bond or chain substitution by alkyl, aryl, aralkyl, (un)saturated hetero(bi)cyclic; R, R' = H (when m ≠ 0), OH, SH, cyano, alkoxy, (un)substituted aryloxy or aralkoxy, cycloalkyl, (un)substituted (un)saturated hetero(bi)cyclic, (un)substituted aryl or aralkyl; or NRR' = (un)substituted N-heterocycle; R3 = COR3', CONHR3', CSNHR3', or SO2R3'; R3' = alkyl; aryl, aralkyl, or (un)saturated hetero(bi)cyclic; including isomers, racemates, enantiomers, diastereomers, and acid and base addition salts]. The compds. are useful for treatment of disorders linked to proteases and kinases, and particularly those in which cathepsin K is implicated. These include cardiovascular diseases, cancers, CNS disorders, inflammatory diseases, infectious diseases, and bone disorders. A list of 47 compds. I is given, as well as a general preparative route to I. Claims include combinatorial libraries of I. For example, compound II was prepared in several steps from a Z-protected hexahydropyridazic acid derivative, Z-protected β-alanine, isovaleric anhydride, a corresponding diazo ketone, and a pyridinedicarboxylic acid derivative Fourteen compds. I, including II, inhibited cathepsin K in vitro, with IC50 values < 1 μM.

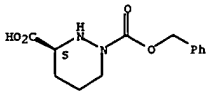
IT **65632-62-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of new pyridazinecarboxylic acid derivs. as inhibitors of cathepsin K)

RN 65632-62-4 CAPLUS

CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

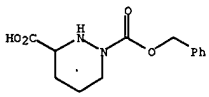
L4 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
cyclocondensation reaction of 2,5-dihalopentanoate esters with dialkyl hydrazodicarboxylates)

RN 72120-54-8 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:581852 CAPLUS
DOCUMENT NUMBER: 135:137513
TITLE: Process for preparing piperazic acid and its derivatives from the cyclocondensation reaction of 2,5-dihalopentanoate esters with dialkyl hydrazodicarboxylates
INVENTOR(S): Brieden, Walter; O'Murchu, Colm
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001056997	A1	20010809	WO 2001-EP1159	20010202
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, US, US				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: EP 2000-102420 A 20000204
US 2000-203936P P 20000512
OTHER SOURCE(S): CASREACT 135:137513; MARPAT 135:137513
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

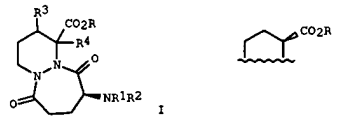
AB Piperazic acid derivs. [I; R1 = C1-20 alkyl; R2 = H, C1-6 alkyl, C1-6 haloalkyl, C1-6 alkoxy, allyloxy, 2,2,2-trichloroethoxy, 2-iodoethoxy, (un)substituted Ph, benzyloxy, 4-methoxybenzyloxy, 2,4-dimethoxybenzyloxy] (e.g., tri-Et hexahydro-1,2,3-pyridazinetricarboxylate) are prepared in high yield and selectivity by the cyclocondensation reaction of a 2,5-dihalopentanoate esters XCH2CH2CH2CHXCO2R1 (X = Br, Cl; e.g., Et 2,5-dibromopentanoate) in the presence of a base (e.g., sodium hydride) and a hydrazodicarboxylate esters R2CONHNHCOR2 (e.g., di-Et hydrazodicarboxylate), followed by basic (e.g., aqueous KOH solution reflux) removal of the blocking groups to give alkali piperazic acid salts (II; M = alkali metal; e.g., piperazic acid potassium salt) followed by amidation with chloroformate esters R3O2CCl (R3 = alkyl, allyl, 2,2,2-trichloroethyl, 2-iodoethyl, benzyl, 4-methoxybenzyl, 2,4-dimethoxybenzyl; e.g., benzyl chloroformate) to form piperazinic acid derivs. [III; N1-(benzyloxycarbonyl)piperazic acid].

IT **72120-54-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for preparing piperazic acid and its derivs. from the

L4 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:739612 CAPLUS
DOCUMENT NUMBER: 132:3373
TITLE: Preparation of (S)-9-amino-3,4,7,8,9,10-hexahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepine-1-carboxylates as pharmaceutical intermediates
INVENTOR(S): Brion, Francis; Crocq, Veronique; Roussel, Patrick
PATENT ASSIGNEE(S): Hoechst Marion Roussel S. A., Fr.
SOURCE: Fr. Demande, 18 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2777888	A1	19991029	FR 1998-5242	19980427
FR 2777888	B1	20040716		
JP 2000001489	A2	20000107	JP 1999-105457	19990413
US 6258947	B1	20010710	US 1999-296325	19990422
EP 955310	A1	19991110	EP 1999-401019	19990426
EP 955310	B1	20041013		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 279434	E	20041015	AT 1999-401019	19990426
PT 955310	T	20050131	PT 1999-401019	19990426
ES 2229641	T3	20050416	ES 1999-401019	19990426
US 2001002422	A1	20010531	US 2001-765761	20010119
US 6433164	B2	20020813		

PRIORITY APPLN. INFO.: FR 1998-5242 A 19980427
US 1999-296325 A1 19990422
OTHER SOURCE(S): CASREACT 132:3373; MARPAT 132:3373
GI



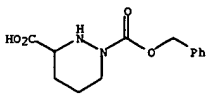
I II

AB Title compds.[I; R = H or (ar)alkyl; R1 = acyl protecting group and R2 = H or R1R2 = atoms to complete a cyclic protecting group] were prepared as intermediates for pyridazinodiazepines II. Thus, I (R1R2 = phthaloyl)(III; R3 = R4 = H)(preparation given) was treated with (Me2CH)2NLi/PhSeBr to give III (R3R4 = bond) which was hydrogenated to give II.

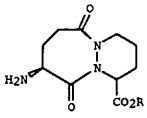
IT **72120-54-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (S)-9-amino-3,4,7,8,9,10-hexahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepine-1-carboxylates as pharmaceutical intermediates)

RN 72120-54-8 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester

L4 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



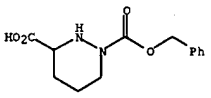
I

AB Title compds. I [R = H, alkyl, aralkyl] in SR configuration or in the form of a SR + SS mixture were prepared Thus, (S,S)-I [R = Me] was obtained from 5-bromopentanoic acid in 8 steps, deracemization being carried out in the last step.

IT **72120-54-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepine-1-carboxylic esters as intermediates for preparing therapeutically active compds.)

RN 72120-54-8 CAPLUS

CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:708785 CAPLUS
DOCUMENT NUMBER: 131:322632
TITLE: Novel octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepine-1-carboxylic acid derivatives as intermediates for preparing therapeutically active compounds
INVENTOR(S): Colladant, Colette; Crocq, Veronique; Larkin, John Patrick; Roussel, Patrick
PATENT ASSIGNEE(S): Hoechst Marion Roussel, Fr.
SOURCE: PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

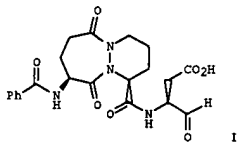
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9955724	A1	19991104	WO 1999-FR981	19990426
W: AE, AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2777889	A1	19991029	FR 1998-5243	19980427
FR 2777889	B1	20040709		
CA 2330492	AA	19991104	CA 1999-2330492	19990426
AU 9934274	A1	19991116	AU 1999-34274	19990426
AU 755286	B2	20021205		
BR 9910020	A	20010109	BR 1999-10020	19990426
EP 1073673	A1	20010207	EP 1999-915834	19990426
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
TR 200003142	T2	20010321	TR 2000-200003142	19990426
JP 2002513030	T2	20020508	JP 2000-545882	19990426
EE 200000619	A	20020617	EE 2000-619	19990426
NZ 507618	A	20030725	NZ 1999-507618	19990426
NO 2000005391	A	20001219	NO 2000-5391	20001026
BG 104891	A	20011031	BG 2000-104891	20001026
HR 2000000733	A1	20010228	HR 2000-733	20001027
ZA 2000006081	A	20011029	ZA 2000-6081	20001027
US 6548664	B1	20030415	US 2000-674327	20001031
HK 1039131	A1	20050513	HK 2002-100645	20020128
US 2002128473	A1	20020912	US 2002-102591	20020320
US 6570012	B2	20030527		
US 2003130269	A1	20030710	US 2002-313422	20021206

PRIORITY APPLN. INFO.: FR 1998-5243 A 19980427
WO 1999-FR981 W 19990426
US 2000-674327 A3 20001031

OTHER SOURCE(S): MARPAT 131:322632
GI

L4 ANSWER 10 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:386128 CAPLUS
DOCUMENT NUMBER: 131:144580
TITLE: An efficient stereoselective synthesis of [3S(1S,9S)]-3-[[[9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxobutanoic acid, an interleukin converting enzyme (ICE) inhibitor
AUTHOR(S): Chen, M. H.; Goel, O. P.; Hyun, J.-W.; Magano, J.; Rubin, J. R.
CORPORATE SOURCE: Parke-Davis Pharmaceutical Research Division, Warner-Lambert Company, Ann Arbor, MI, 48105, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(11), 1587-1592
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

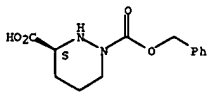
AB The title compound (I) is a potent interleukin-1β-converting enzyme inhibitor. Recently, an efficient chiral synthesis of I was accomplished in our labs. The overall yield of this 18-step stereoselective synthesis was 9.8%.

IT **65632-62-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation of interleukin converting enzyme inhibitor)

RN 65632-62-4 CAPLUS

CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:502830 CAPLUS
DOCUMENT NUMBER: 127:122000
TITLE: Inhibitors of interleukin-1β converting enzyme
INVENTOR(S): Batchelor, Mark J.; Bebbington, David; Bemis, Guy W.; Fridman, Wolf Herman; Gillespie, Roger J.; Golec, Julian M. C.; Gu, Yong; Lauffer, David J.; Livingston, David J.; Matharu, Saroop S.; Mullican, Michael D.; Murcko, Mark A.; Murdoch, Robert; Nyce, Philip L.; Robidoux, Andrea L. C.; et al.
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 946 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9722619	A2	19970626	WO 1996-US20843	19961220
WO 9722619	A3	19971016		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 6008217	A	19991228	US 1995-575641	19951220
US 5874424	A	19990223	US 1996-598332	19960208
US 5985863	A	19991116	US 1996-712878	19960912
US 6204261	B1	20010320	US 1996-761483	19961206
CA 2239904	AA	19970626	CA 1996-2239904	19961220
AU 9715222	A1	19970714	AU 1997-15222	19961220
AU 735075	B2	20010628		
EP 869967	A2	19981014	EP 1996-945318	19961220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9612258	A	19990713	BR 1996-12258	19961220
NZ 326610	A	20000825	NZ 1996-326610	19961220
JP 2002507961	T2	20020312	JP 1997-523098	19961220
TW 541309	B	20030711	TW 1996-85115799	19961220
RU 2249598	C2	20050410	RU 1998-113931	19961220
NO 9802597	A	19980812	NO 1998-2597	19980605
AU 756253	B2	20030109	AU 2001-76122	20010928

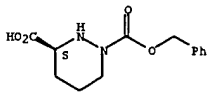
PRIORITY APPLN. INFO.:

US 1995-575641	A	19951220
US 1996-598332	A	19960208
US 1996-712878	A	19960912
US 1996-31495P	P	19961126
US 1996-761483	A	19961206
AU 1997-15222	A3	19961220
WO 1996-US20843	W	19961220

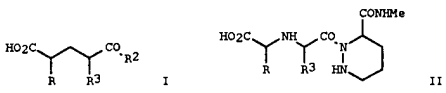
OTHER SOURCE(S): MARPAT 127:122000
AB Compds. R(CH2)nCH(NHR1)(CR22)mR3 [R = NC, R4CH:CH, R4ON:CH, R4CR22, etc.

L4 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
where R2 is independently selected from H, OH, F and R4 is (un)substituted alkyl; R1 = R5NHCHR6CONR7CHR8CO, where CHR6CONR7 is a 2-oxoazepine ring substituted by benzo, pyrido, thieno, or related rings at the 6,7-position and optionally may have O, NH, S, SO, or SO2 at the 5-position, R5 and R8 are H, cyclic group, etc.; R3 = OH, COCOCO2H, CO2H, or any bioisosteric replacement for CO2H; m = 0, 1, 2; n = 0, 1] were prepd. as inhibitors of interleukin-1β converting enzyme. Thus, [1S,9S(2RS,3S)]-9-benzoylamino-6,10-dioxo-1,2,3,4,7,8,9,10-octahydro-N-(2-benzyloxy-5-oxotetrahydrofuran-3-yl)-6H-pyridazino[1,2-a][1,2]diazepine-1-carboxamide was prepd. and shown to have IC50 values of 900 and 600 nM, resp., in the peripheral blood mononuclear cell (PBMC) and whole human blood assays.
IT 65632-62-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(inhibitors of interleukin-1β converting enzyme)
RN 65632-62-4 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

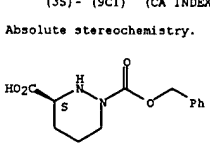


L4 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:468998 CAPLUS
DOCUMENT NUMBER: 127:176690
TITLE: Potent carboxylate inhibitors of stromelysin containing P2' piperazic acids and P1' biaryl moieties
AUTHOR(S): Cherney, Robert J.; Decicco, Carl P.; Nelson, David J.; Wang, Li; Meyer, Dayton T.; Hardman, Karl D.; Copeland, Robert A.; Arner, Elizabeth C.
CORPORATE SOURCE: The DuPont Merck Pharmaceutical Co., Experimental Station, Wilmington, DE, 19880-0500, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1997), 7(13), 1757-1762
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Several carboxylate derivs. I [R = Me, butyl; R2 = L-Tyr(Me)NHMe; R3 = 4-R1-C6H4(CH2)2; R1 = H, Ph] and II [X = CH2, NH; R = Me, butyl; R3 = 4-R1-C6H4W(CH2)2; R1 = Ph, benzyl, pentyl, iso-Pr, butyl; W = bond, O] were synthesized and evaluated as stromelysin (MMP-3) inhibitors. Compds. containing a biphenyl moiety, i.e. R1 = Ph, were found to be potent inhibitors of MMP-3. An X-ray crystal structure of the most potent compound, carboxylate I [R = Bu, R2 = L-Tyr(Me)NHMe, R3 = 4-Ph-C6H4(CH2)2], revealed an important interaction between the inhibitor's biphenyl moiety and histidine 224 in the S1' pocket of MMP-3.
IT 65632-62-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of potent carboxylate inhibitors of stromelysin containing piperazic acids and biaryl moieties)
RN 65632-62-4 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

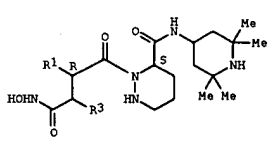
L4 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:194708 CAPLUS
DOCUMENT NUMBER: 124:232477
TITLE: Preparation of hydroxamic acid derivatives as metalloproteinase inhibitors
INVENTOR(S): Broadhurst, Michael John; Brown, Paul Anthony; Johnson, William Henry
PATENT ASSIGNEE(S): F. Hoffmann-la Roche AG, Switz.
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9533731	A1	19951214	WO 1995-EP1956	19950523
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, US, UZ, VN				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9526156	A1	19960104	AU 1995-26156	19950523

PRIORITY APPLN. INFO.:

GB 1994-11598	A	19940609
WO 1995-EP1956	W	19950523

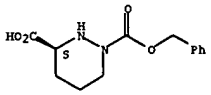
OTHER SOURCE(S): MARPAT 124:232477
GI



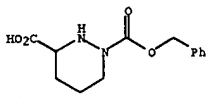
AB R2COCHR1CHR3CONHOH [R1 = C6-12 alkyl; R2 = N-attached heterocyclyl; R3 = (ar)alkyl, heterocyclylalkyl]were prepared Thus, tert-Bu (2R,3RS)-2-heptyl-3-(3-phenylpropyl)hydrogensuccinate was amidated by (3S)-1-benzyloxycarbonyl-3-hexahydropyridazinecarboxylic acid and the product amidated by 4-amino-2,2,6,6-tetramethylpiperidine to give, after further amidation and deprotection, title compound I which had IC50 of 5.7x10-10 and 2.3x10-10M against stromelysin and gelatinase in vitro, resp.
IT 65632-62-4 72120-54-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of hydroxamic acid derivs. as metalloproteinase inhibitors)
RN 65632-62-4 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L4 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



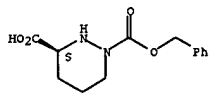
RN 72120-54-8 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester (9CI) (CA INDEX NAME)



L4 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(prepn. of piperazic acid derivs. and analogs as metalloproteinase and tumor necrosis factor inhibitors)

RN 65632-62-4 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

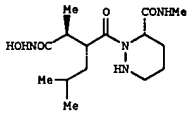


L4 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:150226 CAPLUS
DOCUMENT NUMBER: 124:202303
TITLE: Preparation of piperazic acid derivatives and analogs as metalloproteinase and tumor necrosis factor inhibitors
INVENTOR(S): Decicco, Carl Peter; Jacobson, Irina Cipora; Magolda, Ronald L.; Nelson, David John; Cherney, Robert Joseph
PATENT ASSIGNEE(S): Du Pont Merck Pharmaceutical Co., USA
SOURCE: PCT Int. Appl., 180 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9529892	A1	19951109	WO 1995-US5012	19950427
W: AU, BR, CA, CN, CZ, EE, FI, HU, JP, KR, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, UA, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
ZA 9503399	A	19961028	ZA 1995-3399	19950426
AU 9523947	A1	19951129	AU 1995-23947	19950427
PRIORITY APPLN. INFO.:			US 1994-234195	A 19940428
			US 1995-423193	A 19950418
			WO 1995-US5012	W 19950427

OTHER SOURCE(S): MARPAT 124:202303
GI



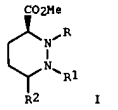
I

AB ACHR2COR [A = NR8CHR9CO2H, CHR11CR9R9aCO2H, CR1R1aCONHOH; R = (un)substituted carbocyclic ring system, -heterocyclyl; R1 = H, halo, alkyl, aryl, heterocyclyl, etc.; R1a = groups cited for R1, NH2, OH, alkoxy, etc.; R2 = (alkoxy)alkyl, (CH2)nOR20, etc.; R8 = H, alkyl, acyl; R9 = H, alk(en)yl, alkynyl; R9a = H, OH, alkoxy, NH2, etc.; R11 = H, alkyl, CH2Ph; R20 = (hetero)aryl, heterocyclyl; n = 0-8) were prepared Thus, (2S,3R)-Me2CHCH2CH(CO2H)CHMeCO2CH2CC13 (preparation given) was amidated by tert-Bu N1-(benzyloxycarbonyl)piperazate and the product converted in 4 steps to title compound I which had Ki of <50nM for inhibition of stromelysin in vitro.

IT 65632-62-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

L4 ANSWER 15 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:131769 CAPLUS
DOCUMENT NUMBER: 125:11384
TITLE: Amino acids and peptides. Part 100. Enantioselective syntheses of (R)- and (S)-hexahydropyridazine-3-carboxylic acid derivatives
AUTHOR(S): Schmidt, Ulrich; Braun, Christine; Sutoris, Heinz
CORPORATE SOURCE: Inst. Org. Chemie Isotopenforschung, Univ. Stuttgart, Stuttgart, D-70569, Germany
SOURCE: Synthesis (1996), (2), 223-9
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:11384
GI



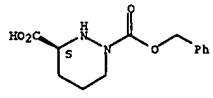
I

AB Pyridazine-3-carboxylic acids e.g. I (R = CO2CH2Ph, R1, R2 = H or bond; R, R2 = H, R1 = CO2CH2Ph) were prepared via ring closure of α-hydrazino- and δ-hydrazinopentanoates. Either optically active glutamic acid or an enantioselective catalytic hydrogenation was used to generate the chiral center. The numerous optically active intermediates are valuable starting materials for the synthesis of other unusual amino acids.

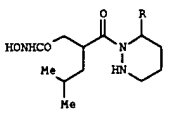
IT 65632-62-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of chiral pyridazinecarboxylic acid derivs. by stereoselective processes)

RN 65632-62-4 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



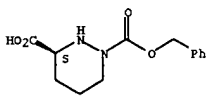
L4 ANSWER 16 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:10651 CAPLUS
DOCUMENT NUMBER: 124:116925
TITLE: Probing the P3' pocket of stromelysin with piperazic acid analogs
AUTHOR(S): Nugiel, David A.; Jacobs, Kim; Decicco, Carl P.; Nelson, David J.; Copeland, Robert A.; Hardman, Karl D.
CORPORATE SOURCE: DuPont Merck Pharmaceutical Co., Wilmington, DE, 19880-0353, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1995), 5(24), 3053-6
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



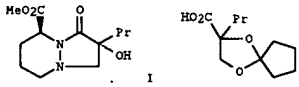
I

AB The piperazic acid analogs I [R = CO2Me, CO2H, CH2OH, CH2OMe] of matlystatin (I, R = CONHMe) were prepared as stromelysin (MMP-3) inhibitors. The methylamide substituent can be replaced by other carboxy-based substituents and maintain good binding affinity. Removal of the hydrogen-bond acceptor results in a 30-fold decrease in activity.
IT **65632-62-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of matlystatin analogs as MMP-3 inhibitors)
RN 65632-62-4 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



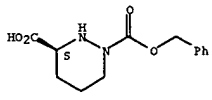
L4 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:956554 CAPLUS
DOCUMENT NUMBER: 124:175991
TITLE: Synthesis of a novel 6,5-bicyclic hexahydropyridazine derivative
AUTHOR(S): Dragovich, Peter S.; Tada, Hiroki; Zhou, Ru
CORPORATE SOURCE: Agouron Pharmaceuticals, Inc., San Diego, CA, 92121, USA
SOURCE: Heterocycles (1995), 41(11), 2487-98
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:175991
GI



I II

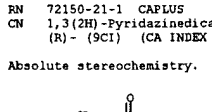
AB A convergent synthesis of the 6,5-bicyclic hexahydropyridazine derivative I is described in which (3S)-N1-Cbz-piperazic acid Me ester is coupled with the functionalized carboxylic acid fragment II. The Sharpless asym. dihydroxylation reaction (AD) of the 1,1-disubstituted olefin EtOCOC(CH2CH2Me):CH2 is utilized in the preparation of II and is observed to produce the corresponding diol with 44% enantiomeric excess and R stereochem.
IT **65632-62-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bicyclic pyridazine)
RN 65632-62-4 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L4 ANSWER 18 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:248180 CAPLUS
DOCUMENT NUMBER: 122:133801
TITLE: Synthetic studies on the azinothricin family of antibiotics. 3. Enantioselective synthesis of a hexapeptide precursor for antitumor antibiotic A83586C
AUTHOR(S): Hale, Karl J.; Delisser, Vern M.; Yeh, Li-Kuan; Peak, S. Andrew; Manaviazar, Soraya; Bhatia, Gurpreet S.
CORPORATE SOURCE: Dep. Chem., Univ. College London, London, WC1H 0AJ, UK
SOURCE: Tetrahedron Letters (1994), 35(41), 7685-8
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:133801
AB A "3+2+1" fragment condensation strategy to a precursor of the hexapeptide found in antibiotic A 83586C is described.
IT **72150-21-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; synthetic studies on azinothricin family of antibiotic and enantioselective synthesis of a hexapeptide precursor for antitumor antibiotic A83586C)
RN 72150-21-1 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (R)- (9CI) (CA INDEX NAME)

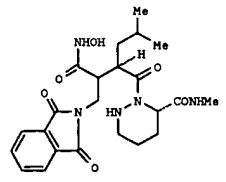
Absolute stereochemistry.



L4 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:700765 CAPLUS
DOCUMENT NUMBER: 121:300765
TITLE: Preparation of oxoheterocyclyl-substituted hydroxamic acid derivatives as collagenase inhibitors
INVENTOR(S): Broadhurst, Michael John; Brown, Paul Anthony; Johnson; William Henry; Lawton, Geoffrey
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 574758	A1	19931222	EP 1993-108628	19930528
EP 574758	B1	19980909		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
US 5318964	A	19940607	US 1993-66832	19930524
AU 9339816	A1	19931216	AU 1993-39816	19930526
AU 659555	B2	19950518		
AT 170840	E	19980915	AT 1993-108628	19930528
ES 2121896	T3	19981216	ES 1993-108628	19930528
ZA 9303957	A	19931213	ZA 1993-3957	19930604
RO 112613	B3	19971128	RO 1993-777	19930604
CZ 283373	B6	19980415	CZ 1993-1081	19930604
IL 105921	A1	19980104	IL 1993-105921	19930607
CA 2098168	AA	19931212	CA 1993-2098168	19930610
NO 9302117	A	19931213	NO 1993-2117	19930610
CN 1083062	A	19940302	CN 1993-107239	19930610
CN 1035616	B	19970813		
JP 06065196	A2	19940308	JP 1993-165228	19930610
JP 07076210	B4	19950816		
FI 109535	B1	20020830	FI 1993-2692	19930611
US 5447929	A	19950905	US 1994-214895	19940317
PRIORITY APPLN. INFO.:			GB 1992-12421 A	19920611
			GB 1993-5720 A	19930319
			US 1993-66832 A3	19930524

OTHER SOURCE(S): MARPAT 121:300765
GI



I

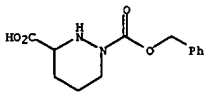
L4 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

AB R1(CH2)nCH(CONHOH)CH(CONR2R3)CHR4CR5R6CH2R7 (R1 = N-attached oxoheterocyclyl; R2 = alkyl; R3 = alkyl or aryl; NR2R3 = heterocyclyl; R4-R7 = H or Me; n = 1-4) were prepared Thus, (2R)-[(1R,S)-tert-butoxycarbonyl-2-phthalimidoethyl]-4-methylvaleric acid was amidated by 1-benzyloxycarbamoyl-(3S)-hexahydropyridazinecarboxylic acid and the product converted in 3 steps to title compound (R,S)-I which had IC50 of 1.2 nM against collagenase in vitro.

IT 72120-54-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of collagenase inhibitor)

RN 72120-54-8 CAPLUS

CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester (9CI) (CA INDEX NAME)



L4 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:408558 CAPLUS

DOCUMENT NUMBER: 119:8558

TITLE: Synthesis and determination of the absolute configuration of matlystatin B

AUTHOR(S): Tamaki, Kazuhiko; Ogita, Takeshi; Tanzawa, Kazuhiko; Sugimura, Yukio

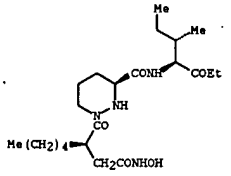
CORPORATE SOURCE: Biosci. Res. Lab., Sankyo Co., Ltd., Tokyo, 140, Japan

SOURCE: Tetrahedron Letters (1993), 34(4), 683-6
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



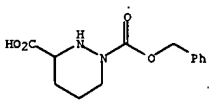
I

AB The title compound was first synthesized and its absolute configuration was determined as I by comparison with the natural product.

IT 72120-54-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(resolution and esterification of)

RN 72120-54-8 CAPLUS

CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester (9CI) (CA INDEX NAME)



L4 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:634509 CAPLUS

DOCUMENT NUMBER: 117:234509

TITLE: Development of a novel class of cyclic hexapeptide oxytocin antagonists based on a natural product

AUTHOR(S): Williams, Peter D.; Bock, Mark G.; Tung, Roger D.; Garsky, Victor M.; Perlow, Debra S.; Erb, Jill M.; Lundell, G. F.; Gould, Norman P.; Whitter, Willie L.; et al.

CORPORATE SOURCE: Dep. Med. Chem., Pharm. Res. Dev., Merck Res. Lab., West Point, PA, 19486, USA

SOURCE: Journal of Medicinal Chemistry (1992), 35(21), 3905-18
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

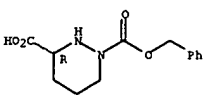
AB Structure-activity profiles for cyclic hexapeptide analogs of oxytocin inhibitor cyclo[L-Pro1-D-Phe2-L-Ile3-D-APiz4-L-APiz5-D-MePhe6) (L-365,209; APiz = dehydropiperazyl) are given. The optimal combination of cyclic amino acid ring sizes at positions 1, 4, and 6 and the role of the N-alkyl substituent at position 6 was elucidated. Lipophilic amino acids at positions 2 and 3 and the unusual amino acid D-APiz at position 4 were the most critical residues for obtaining good oxytocin receptor affinity. Incorporation of amino acids that contain a basic side chain at the less critical 5 and 6 positions maintained good receptor affinity and also provided useful levels of water solubility for i.v. formulation. By combining potency and solubility enhancing substitutions, several analogs were identified that have the desired combination of properties in vitro.

IT 72150-21-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(peptide coupling of, with isoleucine derivative)

RN 72150-21-1 CAPLUS

CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:490798 CAPLUS

DOCUMENT NUMBER: 117:90798

TITLE: Preparation of cyclic hexapeptides as oxytocin antagonists

INVENTOR(S): Bock, Mark G.; Veber, Daniel F.; Tung, Roger D.; Williams, Peter D.; Freidinger, Roger M.

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: Eur. Pat. Appl., 119 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

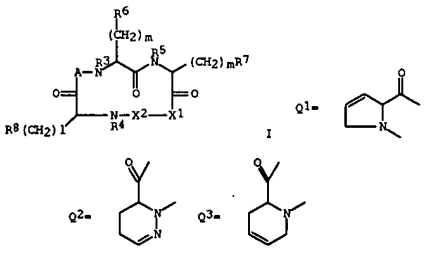
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 444898	A1	19910904	EP 1991-301582	19910227
R: CH, DE, FR, GB, IT, LI, NL				
US 5225528	A	19930706	US 1990-628986	19901217
CA 2036973	AA	19910828	CA 1991-2036973	19910225
JP 05112600	A2	19930507	JP 1991-216769	19910227
PRIORITY APPLN. INFO.:			US 1990-486030 A	19900227
OTHER SOURCE(S):	MARPAT 117:90798			

GI

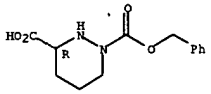


I

AB Title compds. [I; A = Gly, Ala, Ser, MeAla, Q1, etc.; X1 = Ala, Pro, Ser, Thr, Asn, Asp, Glu, Gln, Lys, Arg, His, Orn, 4-hydroxyproline, MeAla, cyclohexylalanine residue, Q2, Q3, etc.; X2 = Q2, Q3, Ala, Pro, Thr, His, cyclohexylalanine, MeAla, 4-hydroxyproline residue, etc.; R3, R4, R5 = H, Me, Et, Pr, allyl, dihydroxypropyl, CH2CO2H; R6 = H, styryl, pyridyl, aminopropyl, benzothienyl, (substituted) Ph, naphthyl, indolyl; R7 = H, Me2CH, Pr, Bu, EtMeCH, cyclopentyl, cyclohexyl, Ph, 4-(PhCH2O)C6H4, 4-HOC6H4, CH2OH, etc.; R8 = H, OH, SH, indolyl, imidazolyl, Ph, naphthyl, aminopropyl, guanidinylethyl, pyridyl, imidazolylalkyl, CONH2, CH2CONH2, etc.; l = 1,2; m = 0-2], were prepared I are useful in treatment of preterm labor and dysmenorrhea, and for stoppage of labor preparatory to caesarian delivery. Thus, cyclo[D-Phe-L-Ile-D-pipecolyl-L-pipecolyl-D-MePhe-L-Pro] was prepared by solid-phase peptide coupling on a phenylacetamidomethyl

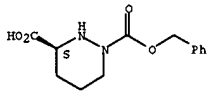
L4 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
resin using fluoroenylmethoxycarbonyl-protected amino acids followed by hydrazinolysis to cleave the resin and cyclization of the resulting hydrazide using isoamyl nitrite in 5N HCl/THF. I inhibited receptor binding of 3H-oxytocin with IC50 = 1.2->10,000 nM.
IT 72150-21-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of cyclic hexapeptide oxytocin antagonists)
RN 72150-21-1 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

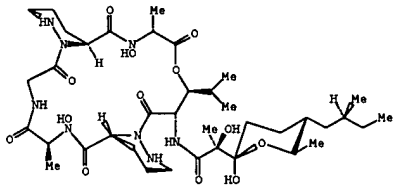


L4 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(coupling of, with glycine deriv.)
RN 65632-62-4 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



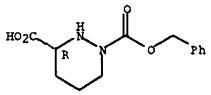
L4 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:631988 CAPLUS
DOCUMENT NUMBER: 113:231988
TITLE: Total synthesis of L-156,602, a novel cyclic hexadepsipeptide antibiotic
AUTHOR(S): Durette, Philippe L.; Baker, Florence; Barker, Peter L.; Boger, Joshua; Bondy, Steven S.; Hammond, Milton L.; Lanza, Thomas J.; Pessolano, Arsenio A.; Caldwell, Charles G.
CORPORATE SOURCE: Dep. Med. Chem. Res., Merck Sharp and Dohme, Rahway, NJ, 07065, USA
SOURCE: Tetrahedron Letters (1990), 31(9), 1237-40
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:231988
GI



I

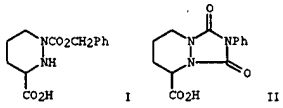
AB The total synthesis of the naturally occurring cyclic hexadepsipeptide antibiotic L-156,602 (I) is described.
IT 72150-21-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with alanine derivative)
RN 72150-21-1 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



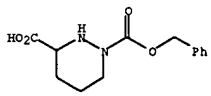
IT 65632-62-4
RL: RCT (Reactant); RACT (Reactant or reagent)

L4 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:423466 CAPLUS
DOCUMENT NUMBER: 111:23466
TITLE: Preparation of 1-(benzyloxycarbonyl)hexahydro-3-pyridazinecarboxylic acid, a protected piperazic acid
AUTHOR(S): Adams, C. E.; Aguilar, D.; Hertel, S.; Knight, W. H.; Paterson, J.
CORPORATE SOURCE: Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA
SOURCE: Synthetic Communications (1988), 18(18), 2225-31
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:23466
GI



I II

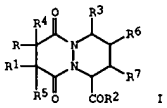
AB 4-Phenylurazole was employed in a multistep synthesis of the title acid (I). The urazole was dehydrogenated, the product underwent a Diels-Alder reaction with CH2:CHCH:CHCO2H, and the adduct obtained was hydrogenated to bicyclic compound II. II was hydrolyzed by KOH, and subsequent acylation with ClCO2CH2Ph gave I.
IT 72120-54-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 72120-54-8 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester (9CI) (CA INDEX NAME)



L4 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1981:532934 CAPLUS
DOCUMENT NUMBER: 95:132934
TITLE: Pyridazopyridazine derivatives, intermediates for their preparation, and their pharmaceutical use
INVENTOR(S): Hassall, Cedric Herbert; Moody, Christopher John
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co. A.-G., Switz.
SOURCE: Eur. Pat. Appl., 51 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 25941	A1	19810401	EP 1980-105411		19800910
EP 25941	B1	19830504			
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE					
AT 3209	E	19830515	AT 1980-105411		19800910
US 4341781	A	19820727	US 1980-186237		19800911
AU 8062357	A1	19810326	AU 1980-62357		19800912
ZA 8005651	A	19810930	ZA 1980-5651		19800912
JP 56081588	A2	19810703	JP 1980-128049		19800917
HU 24145	O	19821228	HU 1980-2284		19800917
HU 181741	B	19831128			
DK 8003958	A	19810320	DK 1980-3958		19800918
FI 8002940	A	19810320	FI 1980-2940		19800918
NO 8002771	A	19810320	NO 1980-2771		19800918
ES 495159	A1	19811116	ES 1980-495159		19800918
ES 503580	A1	19820401	ES 1981-503580		19810701
ES 503581	A1	19820401	ES 1981-503581		19810701
ES 503578	A1	19820501	ES 1981-503578		19810701
ES 503579	A1	19820501	ES 1981-503579		19810701
ES 503582	A1	19820516	ES 1981-503582		19810701
PRIORITY APPLN. INFO.:			GB 1979-32531	A	19790919
			GB 1980-22701	A	19800711
			GB 1979-32431	A	19790919
			JP 1979-32531	A	19790919
			EP 1980-105411	A	19800910

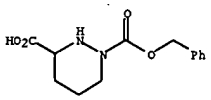
GI



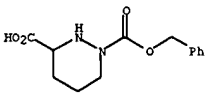
I

AB The antihypertensive compds. I [one of R, R1 = H, alkyl, the other = ZSR8

L4 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(Z = alkylene, R8 = H, alkyl, aryl, acyl, aroyl); R2 = OH, alkoxy, NH2; R3 = H, alkyl aryl; R4-R7 = H; R4R5 and/or R6R7 = bond] were prepd. Thus, (±)-Me 1-(benzyloxycarbonyl)hexahydro-3-pyridazinecarboxylate reacted with AcSCH2CH(COCl)CH2CO2Ph and NaOH in CH2Cl2, followed by treatment with Br in HOAc, then with PCl5 in DMF to give (±)-I (R = R3 = R7 = H, R1 = AcSMe, R2 = Me) (2 diastereomers), which was saponified to I (R = R2 = R3 = R7 = H, R1 = CH2SH), which at 6.25 + 10-8 M gave 50% inhibition of cleavage of hippuryl-histidyl-leucine by angiotensin converting enzyme.
IT 72120-54-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of)
RN 72120-54-8 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester (9CI) (CA INDEX NAME)

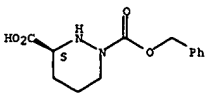


L4 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1980:6901 CAPLUS
DOCUMENT NUMBER: 92:6901
TITLE: Amino-acids and peptides. Part 21. Synthesis of a congener of the cyclohexadepsipeptide antibiotic, monamycin
AUTHOR(S): Hassall, Cedric H.; Johnson, William H.; Theobald, Colin J.
CORPORATE SOURCE: Roche Prod. Ltd., Welwyn Garden City, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1979), (6), 1451-4
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The preparation of monamycin X (I), which differs from natural congeners such as monamycin B3 in that the 3S,5S-5-hydroxypiperazic acid residue is replaced by 3S-piperazic acid (s-Pip), is described. The final synthetic step involves intramol. cyclocondensation reaction of D-Val-L-Ile-R-Pip-S-Pip-N-Me-D-Leu-L-Pro. I exhibited antibacterial activity against Staphylococcus aureus.
IT 72120-54-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and resolution of)
RN 72120-54-8 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester (9CI) (CA INDEX NAME)



IT 65632-62-4P 72120-55-9P 72150-21-1P
72173-00-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate in monamycin congener preparation)
RN 65632-62-4 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



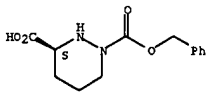
RN 72120-55-9 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (S)-, compd. with [R-(R*,S*)]-α-[1-(methylamino)ethyl]benzenemethano l (1:1) (9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CM 1

CRN 65632-62-4
CMF C13 H16 N2 O4

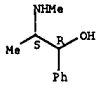
Absolute stereochemistry. Rotation (-).



CM 2

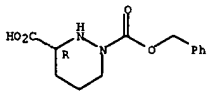
CRN 299-42-3
CMF C10 H15 N O

Absolute stereochemistry.



RN 72150-21-1 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



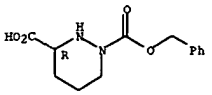
RN 72173-00-3 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (R)-, compd. with (S-(R*,S*))-α-[1-(methylamino)ethyl]benzenemethano l (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 72150-21-1
CMF C13 H16 N2 O4

Absolute stereochemistry.

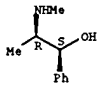
L4 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CM 2

CRN 321-98-2
CMF C10 H15 N O

Absolute stereochemistry. Rotation (+).



L4 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1978:191391 CAPLUS
DOCUMENT NUMBER: 88:191391
TITLE: Synthesis of a congener of the cyclohexadepsipeptide antibiotic monamycin
AUTHOR(S): Hassall, Cedric H.; Johnson, William H.; Theobald, Colin J.
CORPORATE SOURCE: Roche Prod. Ltd., Welwyn Garden City, UK
SOURCE: Journal of the Chemical Society, Chemical Communications (1977), (18), 635-6
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Deoxymonamycin B3 (I), which contains residues of D-valine, L-isoleucic acid, D- and L-hexahydropiperazic acid, N-methyl-D-leucine, and L-proline, was prepared from the protected individual amino acids. I has antibacterial activity against Staphylococcus aureus similar to that of monamycin.

IT 65632-62-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling reaction of, in monamycin congener preparation)

RN 65632-62-4 CAPLUS
CN 1,3(2H)-Pyridazinedicarboxylic acid, tetrahydro-, 1-(phenylmethyl) ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).